Raman Active High Energy Excitations in URu_2Si_2

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Abstract

We have performed Raman scattering measurements on URu_2Si_2 single crystals on a large energy range up to ~ 1300 cm^{-1} and in all the Raman active symmetries as a function of temperature down to 15 K. A large excitation, active only in the E_g symmetry, is reported. It has been assigned to a crystal electric field excitation on the Uranium site. We discuss how this constrains the crystal electric field scheme of the Uranium ions. Furthermore, three excitations in the A_{1g} symmetry are observed. They have been associated to double Raman phonon processes consistently with *ab initio* calculations of the phonons dispersion.

Keywords: Heavy fermions; Exotic electronic order; URu_2Si_2; Hidden order; Raman spectroscopy; crystal electric field (CEF)

1. Introduction

Despite thirty years of intense experimental and theoretical research, the microscopic nature of the low temperature phase ($T < 17.5$ K) of the heavy fermion compound URu_2Si_2 remains unknown [1, 2]. This so-called Hidden Order (HO) phase emerges in the context of a strong mixing between $5f$ electrons of Uranium atoms and the conduction electrons, which makes its identification particularly difficult. Actually, the valence state of the Uranium ions, configurations U^{3+} ($5f^3$ configuration) and U^{4+} ($5f^2$ configuration) or intermediate, is not clearly established and valence fluctuations have been evoked [3, 4, 5]. Nevertheless many interesting theories have been proposed to explain the nature of HO, among which multipolar orders from quadrupolar to dotriacontapolar [6, 7, 8, 9, 10, 11], local currents [12, 13], unconventional density wave [14, 15] modulated spin liquid [16, 17], dynamical symmetry breaking [18] and hastatic

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order [19] for the most recent ones. Although many theories are based on and proposed crystal field schemes (at least the ground state level), all attempts to measure directly the crystal electric field (CEF) excitations in URu_2Si_2 in the paramagnetic state have failed. Only recently, a low energy excitation (1.7 meV) observed by Raman scattering spectroscopy [20, 21] has been suggested as related to a CEF excitation.

Raman spectroscopy is a powerful tool to address the CEF excitations [22, 23, 24], particularly thanks to the selection rules which provide symmetry dependence of each excitations. Here, using electronic Raman spectroscopy, in addition to the usual phonon modes [25], we report the existence of four high energy excitations in URu_2Si_2. Three of them, seen the A_{1g} symmetry, are assigned to double phonon processes while a broader one, seen only in the E_g symmetry, is associated to a crystal field excitation.

2. Methods

Polarized Raman scattering has been performed in quasi-backscattering geometry with the 532 nm line of a solid state laser. We have used a closed-cycle ^{4}He cryostat with sample in high vacuum (10^{-6} mbar). By comparing Stokes and anti-Stokes Raman spectra and via the evolution of phonon frequencies with incident laser power, we have estimated the laser heating of the samples at +1 K/mW. The scattered light has been filtered by RazorEdge filter and analyzed by a Jobin Yvon T64000 spectrometer in a simple grating configuration. All spectra are corrected by the Bose factor. URu_2Si_2 single crystals were grown by the Czochralski method using a tetra-arc furnace [26]. We have used the same samples, polished or freshly cleaved, as in our previous studies [27, 25, 20]. By combining different incident and scattered light polarizations and sample geometries, we have measured the A_{1g}, A_{2g}, B_{1g}, B_{2g} and E_g symmetries (Mulliken-Herzberg notation) of the D_{4h} point group (space group n°139) [28] corresponding respectively to Γ_1^+, Γ_2^+, Γ_3^+, Γ_4^+ and Γ_5^+ in Bethe's notation. For both notations, "g" (gerade) and "+" (even) designate the respect of the space inversion.

3. Results and discussion

Figure 1 shows Raman spectra of URu_2Si_2 up to 1250 cm^{-1} at 220 K for different symmetries. The intense sharp peaks observed at $\sim$ 161 cm^{-1}, $\sim$ 214 cm^{-1}, $\sim$ 391 cm^{-1} and $\sim$ 433 cm^{-1} which correspond to the B_{1g}, $E_g(1)$, $E_g(2)$ and A_{1g} phonon modes, respectively (See black arrows Fig. 1). Energies of all these phonon modes are consistent with our previous comprehensive study [27, 25]. In [E_g] and [A_{2g} + B_{1g}] symmetries, a weak leakage of the A_{1g} phonon mode is seen due to a small crystal misalignment. Three new excitations in the [A_{1g} + B_{2g}] symmetry and a broad excitation only in [E_g] symmetry are reported (See respectively, red dot and straight blue arrows on the Figure 1). Very likely, the peaks in the [A_{1g} + B_{2g}] symmetry correspond to double Raman

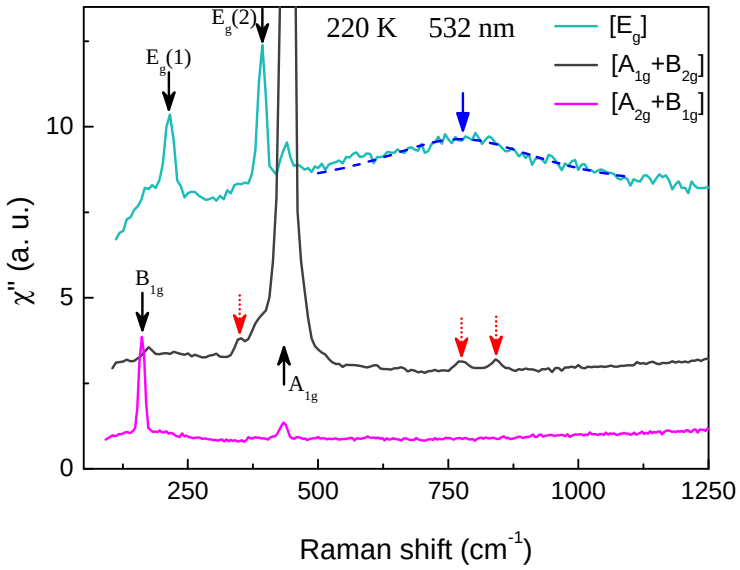

Figure 1: Raman susceptibility in a large energy range in [E_g], [A_{1g} + B_{2g}] and [A_{2g} + B_{1g}] symmetries at 220 K. Black arrows point to the simple-process phonon modes in each symmetry. Four other peaks are observed: three in the [A_{1g}] symmetry (red dotted arrow) assigned to double-process phonon modes, and one in the [E_g] symmetry (blue straight arrow). It is attributed to a CEF excitation on the Uranium ions. The blue dashed line corresponds to a Lorentzian fit of this broad E_g excitation.

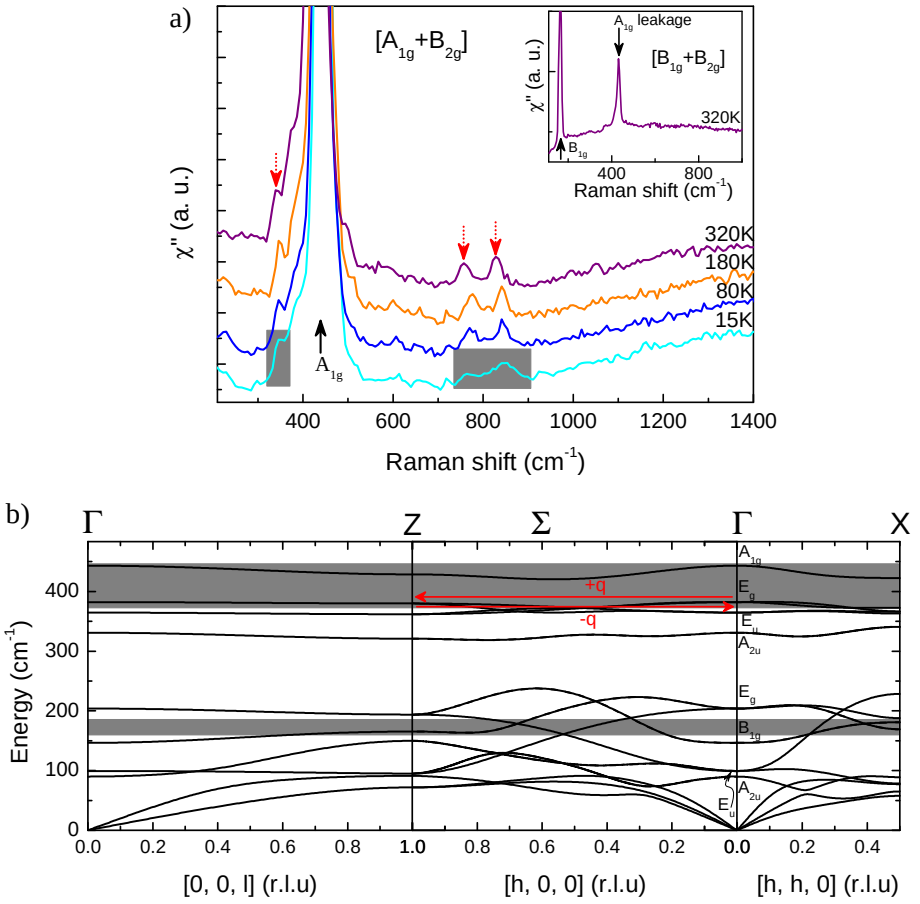

Figure 2: a) Raman susceptibility in the [A_{1g} + B_{2g}] symmetry at various temperatures. Spectra have been shifted for clarity. Inset : Raman spectrum in the [B_{1g} + B_{2g}] symmetry. Simple phonon modes are denoted by black arrow. Red dot arrows point the three double phonon peaks which are of pure A_{1g} symmetry. The grey areas indicate the energy range of the double phonon processes. b) *Ab initio* calculations of the phonon dispersion curves along ΓZ, $\Gamma\Sigma Z$ and ΓX directions at 0 K [25]. The electronic structure was optimized including the spin-orbit coupling within the VASP program [29] and the phonon dispersion relations were obtained using the direct method with atomic displacements $u = 0.06$ Å [30]. The two ($\pm\vec{q}$) red arrows along the [h,0,0] direction depict one possible Raman active double phonon process on the "E_g" branch. The energy range of the grey areas shown in a) is reported on the dispersion curves.

phonon processes with a pure A_{1g} symmetry while the peak in E_g symmetry originates from CEF excitation. The following sections describe further these assignments.

3.1. Double phonon processes in the A_{1g} symmetry

Figure 2 a) presents large energy scale Raman spectra in the [A_{1g} + B_{2g}] symmetry for several temperatures down to 15 K. At 320 K, the three new broad peaks are seen respectively at 344, 758 and 829 cm^{-1} with a linewidth of $\sim$ 30 cm^{-1} (See red dotted arrows in Fig. 2 a)). A slight hardening is observed with decreasing temperature. These new excitations are of pure A_{1g} symmetry since they are not observed in the B_{1g} + B_{2g} symmetry (See inset in Fig. 2 a)).

First, we rule out single phonon processes because all the Raman active phonon modes have been already observed and assigned. Most probably, they are signatures of double phonon processes. Indeed, their energy ranges are in good agreement with *ab initio* calculations of the phonon dispersion [25]. As shown in the Figure 2 b), phonon excitations due to a double process (with a total transfered wave-vector that must be zero, i.e. $\vec{Q} = \pm\vec{q} = 0$) can be Raman active along various directions (such as [h,0,0] shown in Fig2 b), their energy ranges (grey areas) match the Raman shift of the three excitations. They can originate from pure or mixed double processes on the B_{1g}, E_g or A_{1g} branches.

3.2. Crystal electric field excitation in the E_g symmetry

A very broad excitation (FWHM = $\sim$ 400 cm^{-1}) is measured at $\sim$ 760 cm^{-1} at room temperature (See Fig.3). As mentioned previously, this broad excitation is observed only in the E_g symmetry (See Fig.1). Upon cooling the sample, the energy of this large excitation slightly increases up to $\sim$ 800 cm^{-1} at 15 K and its width decreases down to $\sim$ 190 cm^{-1}. This E_g excitation, much larger than the three other excitations seen in the A_{1g} symmetry, is unlikely to be due to a double phonon process. We also rule out the possibility of it coming from a fluorescence effect. Indeed, the fluorescence process is independent of the orientation of the polarization of the incident light. This broad excitation vanishes when the orientation of the polarization of the incident light is modified. For instance, we have observed the broad E_g excitation in the $x(\mathbf{y}, z)\bar{x}$ (E_g probed) configuration[1] where x, y, z correspond to the crystallographic axis, whereas it disappears when the polarization of the incident light is turned in the $x(\mathbf{z}, z)\bar{x}$ (A_{1g} probed) configuration. An excitation at the same energy has been extracted by inelastic neutron scattering experiment by Park et al. [31] where $ThRu_2Si_2$ was used as a phonon background material. Indeed, authors report three excitations, one is on line with our observation with energy of 798$\pm$8 cm^{-1} and FWHM = 290$\pm$16 cm^{-1} at 22 K. They claimed this excitation to be a crystal electric field one. Consequently, the broad peak in the E_g symmetry observed directly by Raman scattering is most probably a crystal electric field

[1] Porto's notation: $\boldsymbol{k_i}(\boldsymbol{e_i}, \boldsymbol{e_d})\boldsymbol{k_d}$

(CEF) excitation ($\Gamma_i \longrightarrow \Gamma_f$, where Γ_i has to be a low energy state) from localized $5f$ electrons of Uranium ions. Measuring a CEF excitation with such large width is certainly inherent to the dual character localized/itinerant of the *5f* electrons.

Park et al. claim that their result is consistent with the CEF scheme proposed by Santini and Amoretti's [32], i.e. a transition $\Gamma_3 \longrightarrow \Gamma_4$ transition. However, the $\Gamma_3 \longrightarrow \Gamma_4$ transition is not Raman active in the E_g symmetry. We can rule out this CEF transition. Table 1 provides all Raman active transitions in the E_g symmetry both for an odd and an even number of electrons on the Uranium sites as well as the mapping of the different *5f* states of the Uranium ions. It appears that none of the ground states (Γ_i=Γ_1 to Γ_7) for the Uranium can be excluded. But once it is established, the final state Γ_f of the excitation is constrained in most cases. For example, with a $5f^2$ configuration of the Urnaium ions, if $\Gamma_i = \Gamma_1$ then $\Gamma_f = \Gamma_5$. We also note that, with a $5f^2$ configuration, the state Γ_5 is always involved in the excitation either as Γ_i or Γ_f. In Table 1, all the other Raman active symmetries of the excitations (in addition to the E_g symmetry activity) are presented. Here, the selection rule for the CEF excitation are given in the D_{4h} symmetry which is the local point symmetry of the Uranium site at high temperature. However, upon entering the hidden order state below 17 K, a change of local point symmetry is hypothesized [33]. Then other point groups (D_4, C_{4h}, D_{2d} and D_{2h}) must be considered.

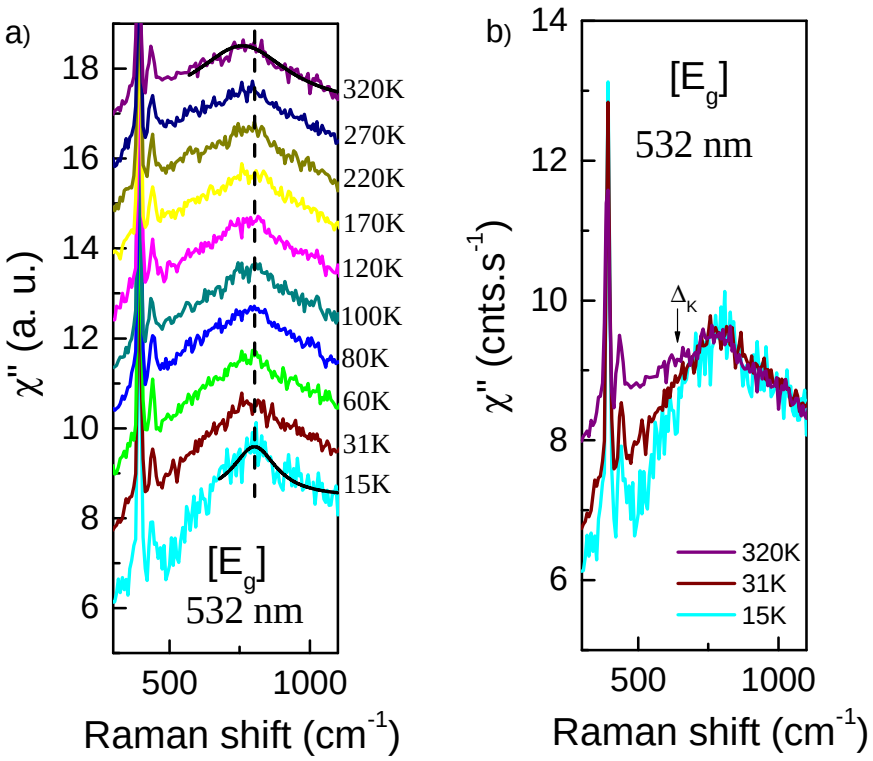

Figure 3: a) Raman susceptibility in [E_g] symmetry at various temperature showing a possible crystal field excitation. The spectra have been shifted vertically. Black curves at 300 K and 15 K are Lorentzian fits. The E_g peak slightly shifts to high energy upon cooling down. b) Raman susceptibility in [E_g] symmetry at 320 K, 31 K and 15 K. Δ_K denotes the energy of closure of the Kondo gap [34].

	Simple irreducible representations *($5f^2$ configuration for U)*				Double irreducible representations *($5f^1$ or $5f^3$ configuration for U)*		
Mapping of the irreducible representations	Γ_1^+ (A_{1g}) Γ_2^+ (A_{2g}) Γ_3^+ (B_{1g}) Γ_4^+ (B_{2g}) Γ_5^+ (E_g)				Γ_6^+ Γ_7^+		
Possible E_g CEF transitions	$\Gamma_5^+ \rightleftarrows \Gamma_1^+$	$\Gamma_5^+ \rightleftarrows \Gamma_2^+$	$\Gamma_5^+ \rightleftarrows \Gamma_3^+$	$\Gamma_5^+ \rightleftarrows \Gamma_4^+$	$\Gamma_6^+ \rightleftarrows \Gamma_6^+$	$\Gamma_6^+ \rightleftarrows \Gamma_7^+$	$\Gamma_7^+ \rightleftarrows \Gamma_7^+$
Additional symmetries of the excitation	None	None	None	None	Γ_1^+, Γ_2^+	Γ_3^+, Γ_4^+	Γ_1^+, Γ_2^+

Possible A_{2g} CEF transitions	$\Gamma_1^+ \rightleftarrows \Gamma_2^+$	$\Gamma_3^+ \rightleftarrows \Gamma_4^+$	$\Gamma_5^+ \rightleftarrows \Gamma_5^+$	$\Gamma_6^+ \rightleftarrows \Gamma_6^+$	$\Gamma_7^+ \rightleftarrows \Gamma_7^+$
Additional symmetries of the excitation	None	None	Γ_1^+, Γ_3^+, Γ_4^+	Γ_1^+, Γ_5^+	Γ_1^+, Γ_5^+

Table 1: List of the CEF excitations localized on the Uranium atoms for even and odd number of *5f* electrons configurations in the D_{4h} local point group symmetry as expected in URu_2Si_2. Are given the excitations which are Raman active in the E_g symmetry (high energy excitation) and the A_{2g} symmetry (low energy excitation [20]). Some of these excitations are active in other symmetries [35].

At present, we cannot give more precise assignment to this high energy CEF transition but it clearly constrains the CEF scheme. The only other observation of a CEF excitation hypothetized so far in URu_2Si_2 is the low energy excitation recently reported in the A_{2g} symmetry at 14 cm^{-1} [20]. Table 1 presents all the CEF transitions compatible with this A_{2g} symmetry. None of these transitions are excluded by our observation in the E_g symmetry. Various CEF schemes are compatible with both observations. For instance, in the $5f^2$ configuration, the A_{2g} excitation may arise from the transition $\Gamma_3 \longrightarrow \Gamma_4$ while the E_g excitation comes from the transition $\Gamma_3 \longrightarrow \Gamma_5$ (see supplementary of [20]). In this case, no other Raman active symmetry are expected for both transitions in the D_{4h} point group. The CEF scheme ($\Gamma_i = \Gamma_2$ and first excited state = Γ_1) proposed by Haule et al. [8] is also compatible with our observations. Furthermore, we do not exclude other kind of multipolar orders [11].

The temperature dependence of the E_g and A_{2g} peaks differ strongly. Indeed, the width of the high energy one (E_g) is roughly constant down to the hidden order transition. Upon entering it below 17 K, the width decreases roughly by a factor 2 and the energy increases slightly by ~ 25 cm^{-1}. However, the error on our fit of the E_g excitation is larger at low temperature than at high temperature because the fitting range is reduced by the opening of the Kondo gap below ~ 700 cm^{-1} [34] (Cf. Fig. 3 b)) and the spectrum at 15 K which have been obtained with less laser power is noisier. On the contrary, the width of the low energy excitation (A_{2g}) diminishes linearly from 300K to 50 K (here the quasi-elastic A_{2g} peak is interpreted as a precursor of the A_{2g} narrow peak of the hidden order state) and it becomes inelastic and much narrower (from 40 cm^{-1} at 50 K to 1 cm^{-1} at 10 K) when entering the HO state [20]. Opening of a gap below $\sim$50 cm^{-1} in the same A_{2g} symmetry may participate to this dramatic change. Although we associate the E_g high energy excitation to a simple CEF excitation, we leave other interpretations on the nature of low energy A_{2g} one open, such as a mode originating from purely itinerant electrons.

4. Conclusion

We have investigated the high energy modes of URu_2Si_2 by Raman scattering. Four new peaks have been observed. Three of them, seen in the A_{1g} symmetry between 300 and 900 cm^{-1}, have been assigned to double phonon processes consistently with the *ab initio* calculations of the phonon dispersion curves. A fourth broad peak observed only in the E_g symmetry at ~ 760 cm^{-1} is attributed to a electric field excitation. This observation constrains the crystal field scheme of the *5f* electrons on the Uranium sites, while allowing for the possibility to consider various CEF scheme, notably ones which are consistent with the interpretation of the low energy A_{2g} excitation as to be due to a CEF excitation.

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